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Published in:
Host Publication

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Document Version
Publisher's PDF, also known as Version of record

Publication date:
2003

[Link to publication in University of Groningen/UMCG research database](#)

Citation for published version (APA):

Nicola, L., van der Giessen, E., & Needleman, A. (2003). Nonlocal Modeling of Size-Dependent Response of Thin Films. In Host Publication Geneva: University of Groningen, The Zernike Institute for Advanced Materials.

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NONLOCAL MODELING OF SIZE-DEPENDENT RESPONSE OF THIN FILMS

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ABSTRACT

A closed-form solution is presented for the plastic response of a single crystal thin film strained by its substrate during thermal loading, according to Gurtin's strain gradient theory [1]. The results are compared with those of discrete dislocation simulations.

INTRODUCTION

The need of an enhanced continuum theory to describe plastic flow at small length scales stems from the incapability of conventional continuum plasticity to capture size effects. Various strain gradient theories have been proposed in the last years, which incorporate length scale effects in different ways, e.g. [1, 2, 3]. We here analyze Gurtin's [1] theory, which is based on the concept of geometrically necessary dislocations, and apply it to solve a boundary value problem for a strained single crystal thin film.

SHORT SUMMARY OF GURTIN'S THEORY

Gurtin [1] has recently developed a strain gradient theory of single-crystal plasticity that accounts for the size dependence arising from geometrically necessary dislocations by including a measure of that density in the expression for the free energy. Here, we confine attention to circumstances where the material response is rate independent and geometry changes are negligible.

The stress rate-strain rate equation is the same used in classical crystal plasticity theory, i.e.

$$\dot{\sigma}_{ij} = \mathcal{L}_{ijkl} \left[\dot{\epsilon}_{kl} - \sum_{\beta} \frac{1}{2} \dot{\gamma}^{(\beta)} \left(s_k^{(\beta)} m_l^{(\beta)} + s_l^{(\beta)} m_k^{(\beta)} \right) \right], \quad (1)$$

where $\dot{\gamma}^{(\beta)}$ is the slip rate on slip system β , as specified by the slip direction $s_i^{(\beta)}$ and the slip plane normal $m_j^{(\beta)}$. The \mathcal{L}_{ijkl} are the linear elastic moduli, which we take to be isotropic and expressed in terms of Young's modulus E and Poisson's ratio ν . The non-local yield condition on slip system β reads

$$\tau^{(\beta)} = \phi^{(\beta)} \text{sign} \dot{\gamma}^{(\beta)} - \xi_{i,i}^{(\beta)}, \quad (2)$$

with $\tau^{(\beta)}$ the resolved shear stress on the slip plane, $\phi^{(\beta)}$ the slip resistance and $(\cdot)_{,i}$ denoting the partial derivative with respect to Cartesian coordinate x_i . The microstress $\xi_i^{(\beta)}$ in (2) is work-conjugate to the slip gradients and is constitutively specified as

$$\xi_i^{(\beta)} = \ell^2 \pi_0 e_{ipq} m_p^{(\beta)} \alpha_{rq} s_r^{(\beta)} \quad (3)$$

where ℓ is a material length parameter, π_0 the initial shear strength and α_{ij} is Nye's dislocation density tensor. The gradient of the microstress, which appears in the yield condition, describes

the so-called energetic hardening related to the energy stored by geometrically necessary dislocations. The slip-system hardening is taken to be local and isotropic so that

$$\dot{\phi}^{(\beta)} = \sum_{\kappa} H_0 |\dot{\gamma}^{(\kappa)}|. \quad (4)$$

In addition to the usual macroscopic boundary conditions, in which either $t_i = \sigma_{ij}n_j$ or u_i are prescribed along the boundary (with outer normal n_i), the strain gradient formulation requires additional so-called microscopic boundary conditions [1], that is, either $\xi_i^{(\beta)}n_i$ or $\gamma^{(\beta)}$ are prescribed at each point of the boundary.

SOLUTION FOR A SINGLE CRYSTAL THIN FILM ON A SUBSTRATE

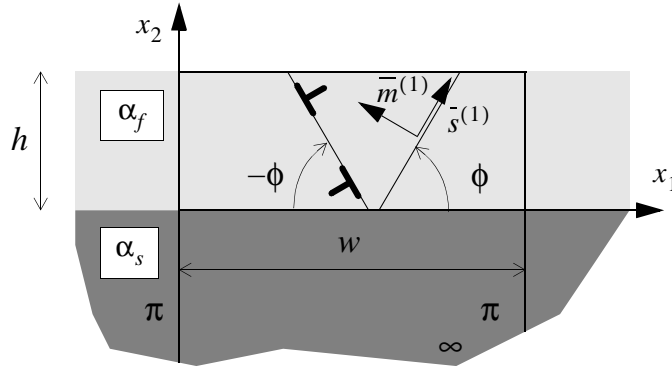


Figure 1: Geometry of the thin film problem in symmetric double slip.

We consider a two-dimensional representation of a single crystal thin film on a semi-infinite substrate, with two symmetrically oriented slip systems (see Fig.1). Plane strain is assumed in the direction perpendicular to the x_1 – x_2 plane. The film is taken to be infinitely long in the x_1 –direction and initially homogeneous. The crystal is oriented for symmetric double slip so that the angle $\phi^{(\beta)}$ between slip plane and film–substrate interface is $\phi^{(1)} = -\phi^{(2)} \equiv \phi$. Then

$$\mathbf{s}^{(1)} = \cos\phi \mathbf{e}_1 + \sin\phi \mathbf{e}_2, \quad \mathbf{m}^{(1)} = -\sin\phi \mathbf{e}_1 + \cos\phi \mathbf{e}_2; \quad (5)$$

$$\mathbf{s}^{(2)} = -\cos\phi \mathbf{e}_1 + \sin\phi \mathbf{e}_2, \quad \mathbf{m}^{(2)} = -\sin\phi \mathbf{e}_1 - \cos\phi \mathbf{e}_2 \quad (6)$$

A quasi-static monotonic thermal loading is imposed by cooling the film–substrate system from an initial temperature T_0 . The substrate undergoes unconstrained contraction but, due to the mismatch between the thermal expansion coefficient of film (α_f) and substrate (α_s), stress develops in the film; tensile for $\alpha_f > \alpha_s$. The macroscopic boundary conditions prescribed are the traction-free conditions at the top of the film:

$$\sigma_{12}(x_1, h) = \sigma_{22}(x_1, h) = 0. \quad (7)$$

The additional microscopic boundary conditions are the micro-free condition at the film top, where dislocations can freely leave the film, and the micro-clamped condition at the film–substrate interface where slip cannot occur, i.e.

$$n_i \xi_i^{(\beta)}(x_1, h) = \xi_2^{(\beta)}(x_1, h) = 0, \quad \gamma^{(\beta)}(x_1, 0) = 0. \quad (8)$$

With all stress components independent of x_1 , equilibrium together with the macroscopic boundary conditions (7) require that $\sigma_{12} = \sigma_{22} = 0$ throughout the film. The elastic solution is a spatially uniform field $\sigma_{11}(x_2) = \text{const.}$, so that yield takes place uniformly in the crystal when $\tau = |\pi_0|$ on both slip systems, with

$$\tau^{(1)} = -\tau^{(2)} = -\frac{1}{2}\sigma_{11} \sin 2\phi \equiv -\tau \quad (9)$$

Because of the double slip orientation and from symmetry considerations,

$$\gamma^{(1)} = -\gamma^{(2)} \equiv -\gamma. \quad (10)$$

From the hardening equation (4), the slip resistance on both slip planes is found as $\phi = \pi_0 + 2H_0\gamma$. Owing to (10), the yield conditions (2) on the two slip systems lead to the same differential equation for $\gamma(x_2)$. The time derivative of this equation can be expressed as

$$\frac{d^2\dot{\gamma}}{dx_2^2} - \frac{4H_0}{\pi_0\ell^2 \sin^2 2\phi} \dot{\gamma} = -\frac{\dot{\sigma}_{11}}{\pi_0\ell^2 \sin 2\phi}. \quad (11)$$

The stress field σ_{11} is not uniform and unknown at this stage. Because of symmetry and because strain rate components do not depend on x_1 , $\dot{\epsilon}_{11}$ must be constant throughout the film. The substrate expands by $(1+\nu)\alpha_s\dot{T}$ so that compatibility of deformation between the film and the substrate requires that $\dot{\epsilon}_{11} = (1+\nu)\alpha_s\dot{T}$. Hence,

$$\dot{\epsilon}_{11} = (1+\nu)\alpha_s\dot{T} = \dot{\epsilon}_{11}^e + \dot{\epsilon}_{11}^p + (1+\nu)\alpha_f\dot{T} \quad (12)$$

so that

$$(1+\nu)(\alpha_s - \alpha_f)\dot{T} = \frac{(1-\nu^2)}{E}\dot{\sigma}_{11} + \dot{\gamma}\sin 2\phi. \quad (13)$$

Solving for $\dot{\sigma}_{11}$ from (11) we obtain the following ordinary second-order differential equation for $\dot{\gamma}$:

$$\frac{d^2\dot{\gamma}}{dx_2^2} - \lambda^2\dot{\gamma} = -F\dot{T} \quad (14)$$

with constant coefficients λ and F given through

$$\lambda^2 = \frac{4H_0}{\pi_0\ell^2 \sin^2 2\phi} + \frac{E}{(1-\nu^2)\ell^2\pi_0}, \quad F = \frac{E(\alpha_s - \alpha_f)}{(1-\nu)\ell^2\pi_0 \sin 2\phi}. \quad (15)$$

Solving this differential equation and making use of the microscopic boundary conditions (8) and (9) we obtain the solution

$$\dot{\gamma} = \frac{(1+\nu)E(\alpha_s - \alpha_f)\sin 2\phi}{4H_0(1-\nu^2) + E\sin^2 2\phi} [1 - \cosh \lambda x_2 + \tanh \lambda h \sinh \lambda x_2] \dot{T}. \quad (16)$$

Substituting this back into (13), we find a linear relation between $\dot{\sigma}_{11}$ and \dot{T} , which after integration with respect to time from the onset of yield (at temperature $T_y < T_0$) to the current temperature T gives

$$\sigma_{11} = \sigma_y + (\sigma_n - \sigma_y)[1 - \beta(1 - \cosh \lambda x_2 + \tanh \lambda h \sinh \lambda x_2)] \quad (17)$$

with

$$\beta = \left[1 + (1 - \nu^2) \frac{4}{\sin^2 2\phi} \frac{H_0}{E} \right]^{-1} \quad (18)$$

Here,

$$\sigma_y = -\frac{E}{1-\nu}(\alpha_f - \alpha_s)(T_y - T_0), \quad \sigma_n = -\frac{E}{1-\nu}(\alpha_f - \alpha_s)(T - T_0) \quad (19)$$

are the (uniform) film stress at the onset of yield (at temperature T_y) and the stress in the absence of plasticity, respectively.

COMPARISON WITH DISCRETE DISLOCATION RESULTS

The problem of a thin film on a semi-infinite substrate as illustrated in Fig.1 has been studied using discrete dislocation (DD) simulations in [4]. In that analysis, the problem is two dimensional, but, afterwards, the resulting σ_{11} fields are averaged along the x_1 direction and denoted by $\langle \sigma_{11} \rangle$ in the sequel. We shall compare here the results for a crystal orientation where $\phi = 30^\circ$.

When cooling from a stress-free and dislocation-free state at $T_0 = 600\text{K}$, the substrate imposes an increasing strain on the film. After an initial elastic response, the first dislocation loop is nucleated and the yield point is reached. Plastic deformation then evolves further with the nucleation and glide of many other dislocations. Results obtained for three different film thicknesses — $h = 1\mu\text{m}$, $h = 0.5\mu\text{m}$ and $h = 0.25\mu\text{m}$ — show that the average in-plane stress in the films at a final temperature of 400K is dependent on the film thickness. The size dependence originates from the large stress gradient at the film-substrate interface, caused by dislocation pile ups. Instead of a uniform stress distribution across the film height, as in the elastic state or according to classical local plasticity, the stress increases as the interface is approached, see Fig. 2a. The vertical lines in this figure indicate the average stress in each film, $\langle \sigma_{11} \rangle_f$. These values are tentatively fitted in Fig. 2b to a power law of the form $\sigma_{11} \propto h^{-p}$; different values of p are required to fit the data for films thinner than $0.5\mu\text{m}$ ($p \cong 0.6$) and for films thicker than $0.5\mu\text{m}$ ($p \cong 1$).

As outlined in the previous section, Gurtin's [1] theory allows for a closed-form equation for the film-average stress as a function of h , by simply integrating (17) over the film thickness. Evidently, we need values for the five material parameters that enter the solution: E , ν , π_0 , H_0 and ℓ . For the elastic constants we take the same characteristic values for aluminum ($E = 70\text{GPa}$ and $\nu = 0.33$) as in the DD simulations [4]. The initial shear strength π_0 is taken from the DD results to be $\pi_0 = 15.5\text{MPa}$. Yield in the DD simulations is determined by the strength of the weakest dislocation source. The values of the source strengths in the simulations are chosen out of a Gaussian distribution with average $\tau_{\text{nuc}} = 25\text{MPa}$ and standard deviation of 5MPa . The dissipative hardening modulus H_0 has no direct counterpart in the DD simulations. In any case, the solution obtained from Gurtin's theory presented above turns out to be practically independent of H_0 for $H_0 < 100\text{MPa}$. We choose $H_0 = 0$, which corresponds to no hardening in a free standing film.

The only parameter left free is the length scale ℓ originating from (3). A value of $\ell = 1.8\mu\text{m}$ gives the $\langle \sigma_{11} \rangle_f$ - h curve which agrees quite well with the DD data points, as shown in Fig. 3b. Figure 3a shows the stress profiles across the film height according to the solution (17). Indeed a stress gradient is predicted, more or less independent of h , as in the DD results of Fig. 2a. According to the solution obtained from Gurtin's theory the stress at the film-substrate interface is the same for all films, independent of h , and equal to the elastic stress σ_n . Figure 4, finally,

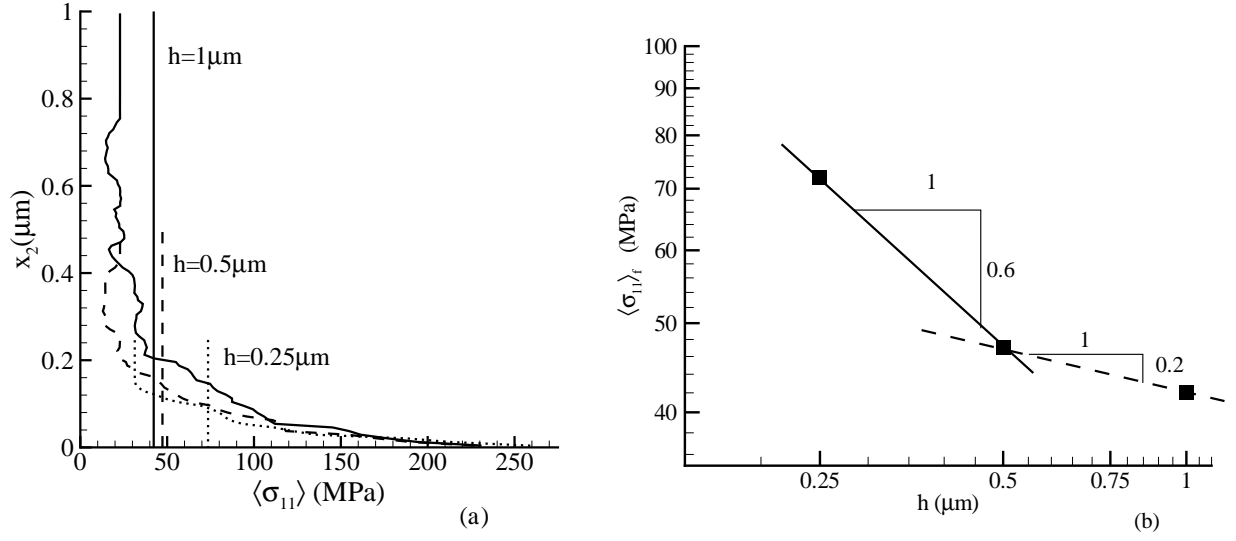


Figure 2: DD results [4] at final temperature. (a) Profiles across the film thickness of the in-plane stress in the films averaged along x_1 . (b) Average film stress versus film thickness with data points being fitted to a power law.

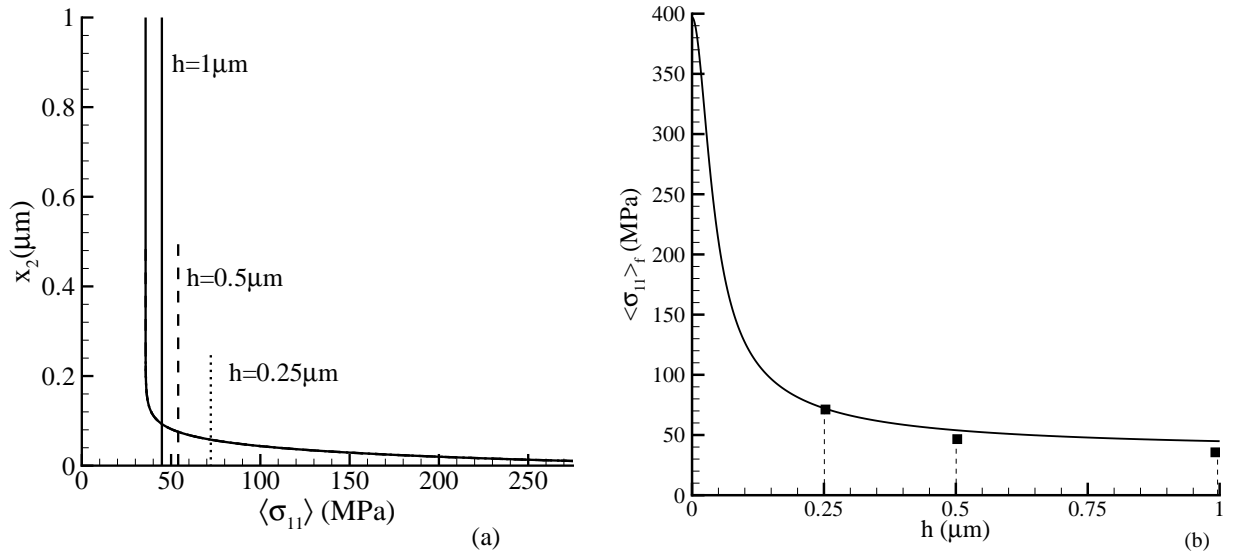


Figure 3: Predictions of Gurtin's theory for $\phi = 30^\circ$ with $\ell = 1.8\mu\text{m}$ at the same final temperature as in Fig. 2. (a) Profiles of the in-plane stress across the film thickness. Vertical lines indicate the average stress in the films, which are plotted in (b) as a function of film thickness h (scaling behavior $\langle \sigma_{11} \rangle_f \propto \tanh \lambda h / \lambda h$). Square symbols indicate the data points from the DD simulations.

shows the stress–temperature curves given by the Gurtin's solution (17). The linear hardening is consistent with the DD results [4].

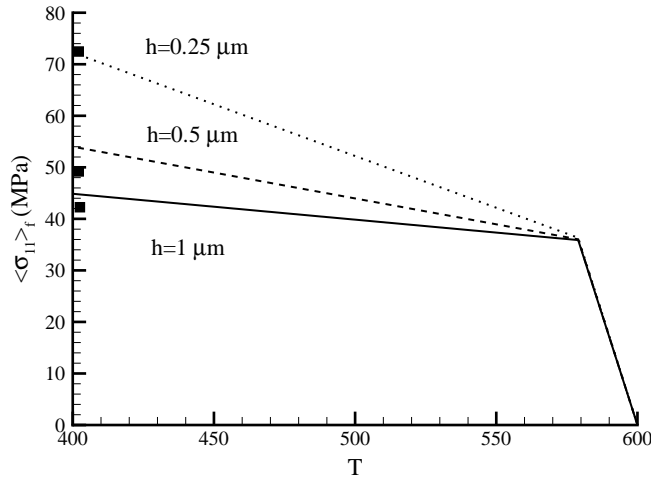


Figure 4: Film-average stress-temperature curves according to the strain gradient solution eq. (17) for $\ell = 1.8\mu\text{m}$ and $\phi = 30^\circ$. Square symbols indicate the stress at final temperature in the DD simulations, as shown also in Figs. 2 and 3.

CONCLUSIONS

A boundary value problem for thermal stress evolution in a single crystal thin film oriented for symmetric double slip has been solved using Gurtin's [1] strain gradient plasticity theory. The material parameters appearing in the solution have been fit to DD results [4] for the same boundary value problem for a crystal with $\phi = 30^\circ$. Both types of calculations give rise to a highly stressed boundary layer near the interface. A reasonably good fit to the DD results is obtained by taking the material length parameter to be $\ell = 1.8\mu\text{m}$ and by neglecting any isotropic hardening — $H_0 = 0$ in (4)— in the slip resistance. This value of ℓ is roughly five times greater than the value obtained by Bittencourt *et al.* [5] by comparison with the DD results of Shu *et al.* [6] for shearing of a single crystal strip between impenetrable walls. A similar comparison between the predictions of Gurtin's nonlocal theory and DD predictions for $\phi = 60^\circ$ did not give a good correspondence. Reasons for the discrepancy with this orientation are being investigated.

ACKNOWLEDGEMENTS

This research was carried out under project number MS97007 in the framework of the Strategic Research program of the Netherlands Institute for Metals Research in the Netherlands (www.nimr.nl).

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